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BOUNDARY CONDITIONS FOR THE PALEOENVIRONMENT: CHEMICAL AND
PHYSICAL PROCESSES IN THE PRE-SOLAR NEBULA

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Current Research

Irvine and graduate student S. Madden, in collaboration with colleagues at the Herzberg Institute of Astrophysics in Canada, continued their study of the first interstellar hydrocarbon ring, cyclopropenylidene (C_3H_2). Both a survey of galactic sources in several C_3H_2 transitions and a more detailed study of a sub-set of these sources are under way. In the latter category is a study of the nearby cold dark cloud TMC-1, which is a potential formation site for solar-type stars. Figure 1 shows spectra of seven rotational transitions which have been observed at the Five College Radio Astronomy Observatory. Three of these have been detected for the first time in any astronomical source: the $3_{30}-2_{21}$ transition at 216 GHz, the $2_{21}-1_{10}$ transition at 122 GHz, and the $1_{11}-0_{00}$ transition at 52 GHz. From the data it is apparent that C_3H_2 is quite spacially extended in typical interstellar molecular clouds, and that at least in TMC-1 it is one of the most abundant organic molecules.

Because it is apparent that many of the C_3H_2 transitions observed in

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C_3H_2 DETECTIONS IN TMC-1

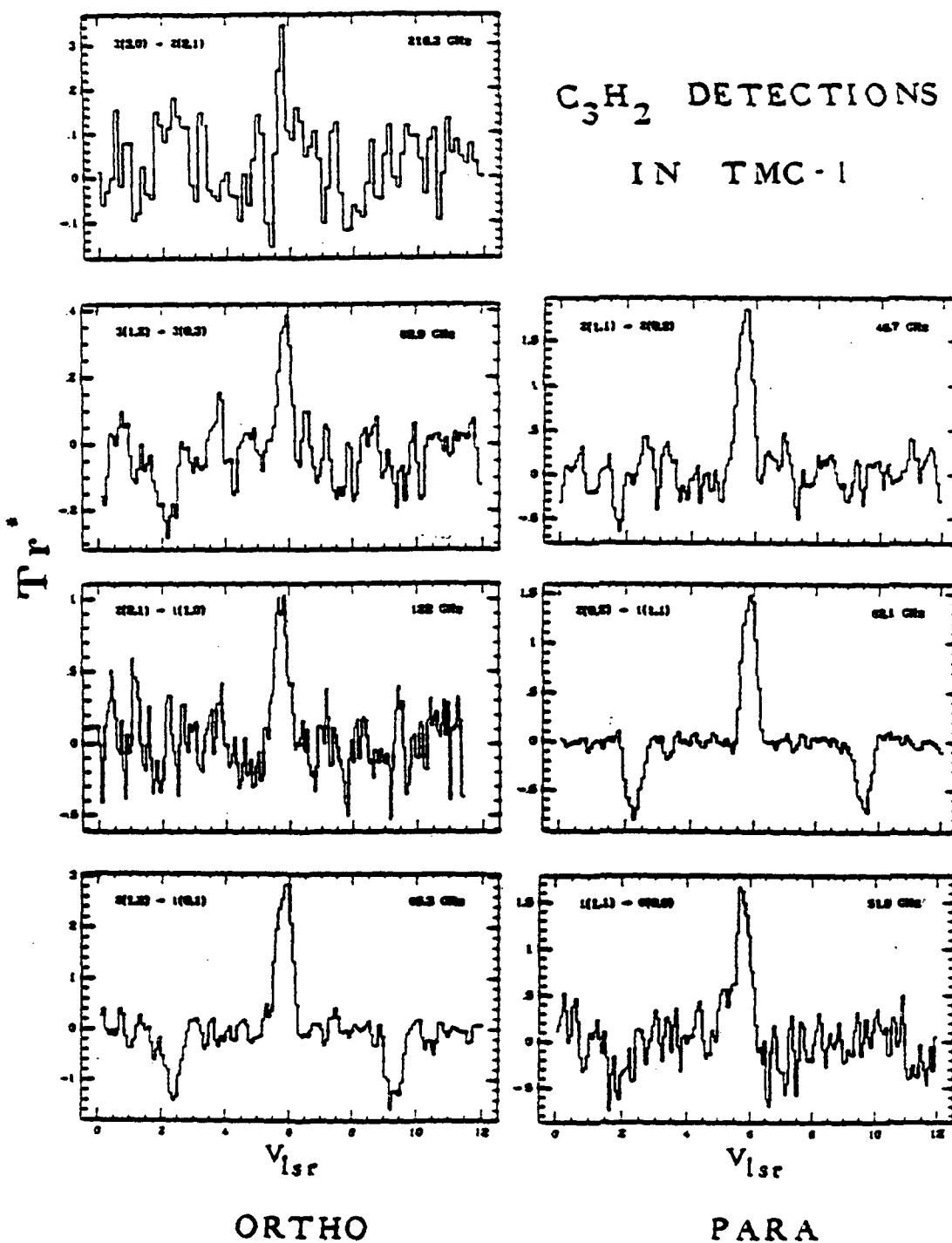


Figure 1 — FCRAO observations of the ring molecule C_3H_2 in the dark cloud TMC-1. First astronomical detections of the 330-221, 221-110, and 111-000 lines. The frequency versatility of the 14m telescope system was critical to this multi-transition study, which spans 46 to 216 GHz.

cold clouds are strongly saturated, observations of rarer isotopic variants are very important in order to establish the true opacity in these lines. This has recently become possible following the measurement of both ^{13}C variants in a molecular spectroscopy laboratory at Lille, France. Following publication of the molecular constants, we have made the first detection of a ^{13}C variant, as shown in Figure 2. Such detections allow estimates to be made of the fractional abundance of the main isotopic variant in three interstellar sources. As expected, C_3H_2 is indeed one of the most abundant organic constituents in the cold cloud TMC-1. It is about an order of magnitude less abundant in the giant molecular cloud Sgr B2, located close to the Galactic center. On the other hand, in the sources observed to date it is most abundant in the envelope of the evolved carbon star IRC+10216. This pattern of abundances is similar to that of the cyanopolyynes, suggesting that the formation mechanisms for C_3H_2 may be related to that for linear carbon chains.

The study of C_3H_2 has also been pursued at other radio observatories where that has been appropriate. For example, the facilities of the National Radio Astronomy Observatory in Green Bank, West Virginia, have been used to investigate the $2_{20}-2_{11}$ transition, which has the surprising property that it is seen in absorption against the cosmic microwave background. This implies that it is "refrigerated" below the universal 3 K background. Since the excitation is thus very far from equilibrium, it seems likely that the behavior of this transition may be a sensitive probe of physical conditions in interstellar sources.

In a continuing study of the chemistry of the cold, quiescent dark clouds, many of which may contain solar mass protostars or presolar nebula, Madden and visiting Swedish astronomer P. Friberg have shown that methanol (CH_3OH) is

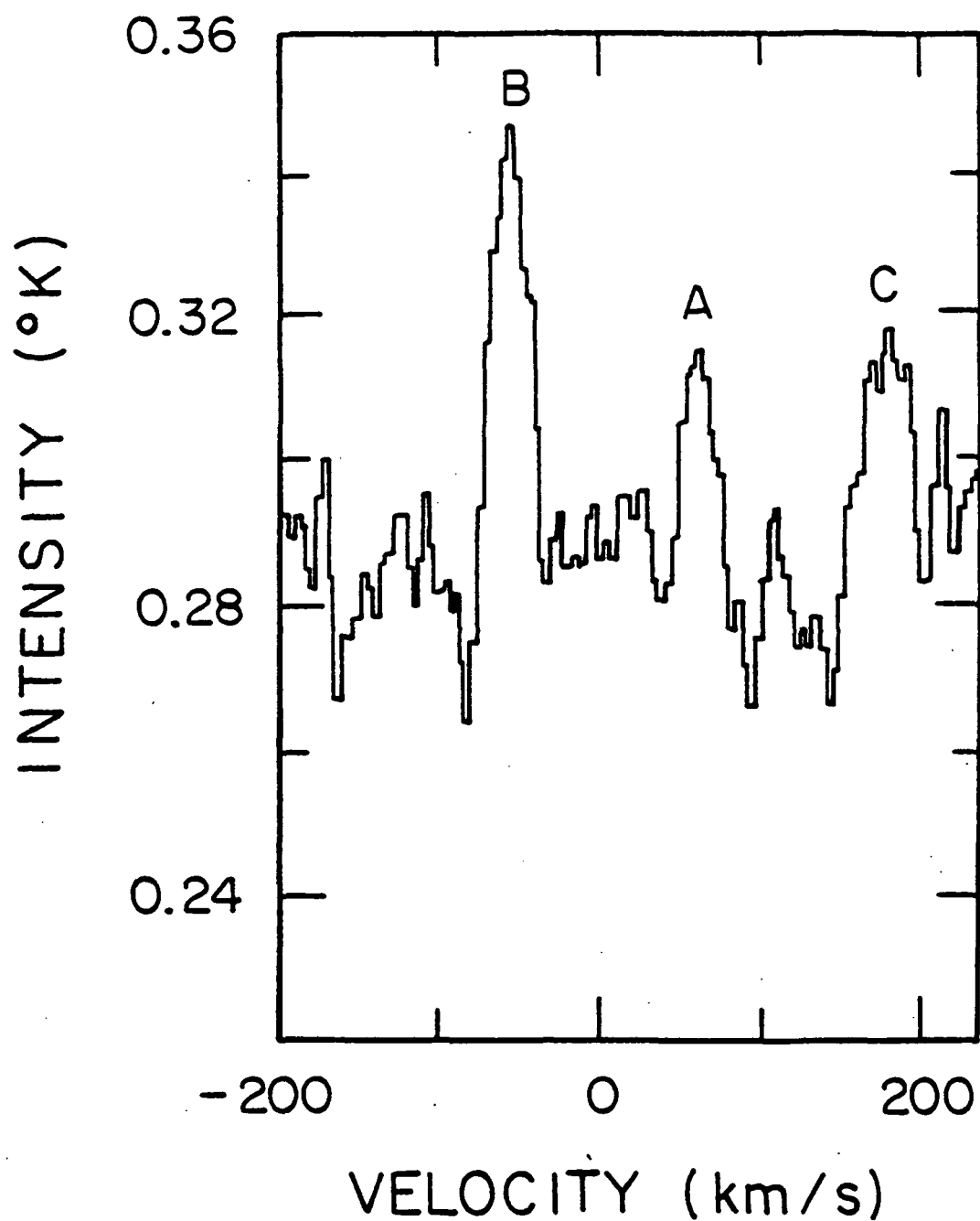


Figure 2 — Spectrum of the Galactic center cloud Sgr B2 at 84 GHz showing emission due to 13 -carbon substituted C_3H_2 (A), CH_3CHO (B), and CH_3CH_2CN (C). Horizontal axis expresses frequency in terms of Doppler velocity relative to the local standard of rest, taking the rest frequency of the observed $2_{12}-1_{01}$ transition of $^{13}CCCH_2$ as 84185-.629 MHz.

widely distributed in such sources. Interestingly enough, this molecule appears to be roughly equally abundant in all of the dark clouds surveyed, unlike the cyanopolyynes, which exhibit very pronounced abundance variations from source to source. In a related search for other oxygen-containing organic molecules, dimethyl ether (CH_3OCH_3) was sought in the dark clouds TMC-1 and L134N, and upper limits on its abundance were obtained.

In a collaboration with radio astronomers in France and at the NRAO, L. Ziurys has made a tentative detection of a new interstellar ion, protonated water (H_3O^+). Only one transition, at 307 GHz, has thus far been detected, so that the assignment must be regarded as tentative until further lines can be sought. Nonetheless, H_3O^+ is an expected constituent of interstellar clouds, and its detection would provide a way to estimate the important abundance of water in these sources. The principal transitions of water itself are in the submillimeter region and are blocked from observations by the Earth's atmosphere.

In a collaboration with scientists from the University of Wisconsin, Irvine and UMass astronomer R. Dickman have discovered another new interstellar ion, SO^+ . This is an important addition to the interstellar inventory, since the chemistry of sulfur-containing molecules in the interstellar medium is a matter of considerable controversy. In particular, there have been suggestions that the abundance of previously detected sulfur-containing species cannot be well explained by existing gas phase models of interstellar chemistry and may require production mechanisms involving the particulate grains. The results of the SO^+ observations are currently being analyzed in order to address these questions.

The study of differences in the chemistry among interstellar clouds is critical for determining the type of processes which take place and the degree

to which chemical evolution occurs as the clouds themselves evolve. Ziurys has been using the FCRAO 14 meter antenna to study "high temperature" chemistry in order to investigate possible differences with respect to that in the cold, quiescent clouds. One approach to this problem is through observations of vibrationally excited species. In order for vibrational excitation to occur, molecules must be present in unusually hot and dense gas, and/or where strong infrared radiation is present. Vibrational excitation thus serves as a probe of physical conditions near star-forming regions and traces material where shock or high temperature chemistry may be occurring. Most recently the emission from vibrationally excited HCN has been mapped in the core of the Orion Molecular Cloud at 267 GHz. The results show that the emission arises from a region smaller than 20 arcseconds. Such a distribution is consistent with the assumption that the molecules are located in the "hot core" component of this cloud, and the abundance can be compared with that of other constituents detected in this region.

A number of molecules containing second and third row elements from the periodic table are thought to be formed from high temperature processes and/or the destruction of interstellar grains. If the gas is sufficiently hot, activation energy barriers in chemical reactions may be overcome, allowing otherwise inaccessible reaction pathways to take place. Ziurys has been continuing her study of SiO and SiS in this regard and appears to have discovered a possible new protostar in the Orion Molecular Cloud. In addition to these silicon-containing species, searches have been made for molecules containing other second and third row elements, including MgO, CaOH, and PN. Emission lines which may be assignable to PN have been detected in several sources. There are also lines that may arise from CaOH, although positive identification of this species awaits a better determination of laboratory

rest frequencies.

Irvine and Ziurys continue their efforts to identify a harmonically related series of interstellar emission lines occurring in both the cold cloud TMC-1 and in the giant molecular cloud Sgr B2. Stringent upper limits to lines at intermediate frequencies have been obtained, so that the quantum numbers of the observed transitions can now be specified. As a result, an approximate rotational constant has been determined.

Schloerb and colleagues at the University of Massachusetts have continued their study of the detailed structure of molecular material in regions of active star formation. It is clear that the formation of both solar type and more massive stars is typically accompanied by violent outflows of material which can disrupt the surrounding ambient cloud, perhaps terminating the process of star formation. Study of this process involves high spacial resolution mapping of extended regions of such clouds, and recent efforts of concentrated on the Orion Molecular Cloud.

Irvine presented invited reviews on interstellar chemistry at the COSPAR meeting in Toulouse, France, in early July of this year, and a more extended review at a Summer School on Interstellar Processes organized by the University of Wyoming and the American Astronomical Society, also in July of 1986. Irvine also continues as Co-chairman of a series of NASA Workshops on Exobiology in Earth Orbit and has been assisting in the editing of the Workshop Report. Ziurys and Schloerb attended the Summer School on Interstellar Processes in Wyoming and presented papers on research relevant to this grant.

Papers supported by this grant and published during the period of this report:

1. "Observations of the Hydrocarbon Ring C_3H_2 ", Matthews, H.E. and Irvine, W.M., in Masers, Molecules and Mass Outflows in Star

Forming Regions, ed. A. Haschick (NEROC Haystack Obs.), pp. 1-8 (1986).

2. "Boundary Conditions for the Paleoenvironment: Chemical and Physical Processes in Dense Interstellar Clouds", Irvine, W.M., Schloerb, F.P. and Ziurys, L.M., in Second Symp. Chem. Evol. and Origin of Life, NASA Conf. Publ. 2425, p. 42.
3. "Ammonia Masers Detected in Star-Forming Regions", Madden S.C., Irvine, W.M., Matthews, H.E., Brown, R.D., and Godfrey, P.D., in Masers, Molecules and Mass Outflows in Star Forming Regions, ed. A. Haschick (NEROC Haystack Obs.), pp. 289-298 (1986).
4. "HCNH⁺: A New Interstellar Molecular Ion", Ziurys, L.M., and Turner, B.E., Ap.J. (Letters), 302, L31 (1986).
5. "New Detections of Interstellar Transient Molecules", Ziurys, L.M., and Turner, B.E., 17th International Symposium on Free Radicals and other Transient Species, Granby, CO, August 1985.
6. "Vibrationally-Excited HCN in Orion-KL and IRC+10216", Ziurys, L.M., and Turner, B.E., Molecules, Masers, and Mass Outflows in Star Forming Regions, ed. A. Haschick (NEROC Haystack Obs.), pp. 23-30 (1986).

Research supported by this grant currently in press:

1. "Variations in the HCN/HNC Abundance Ratio in the Orion Molecular Cloud", Goldsmith, P.F., Irvine, W.M., Hjalmarson, Å., and Ellender, J., Astrophys. J., in press (1986).
2. "Studies of Organic Molecules Containing Methyl Groups in Dark Clouds", Friberg, P., Irvine, W.M., Madden, S.C., Hjalmarson, Å., in Astrochemistry (IAU Symp. 120), ed. M.S. Vardya and S.P. Tarafdar (D. Reidel), in press (1986).
3. "The Chemistry of Cold Dark Interstellar Clouds", Irvine, W.M., in Astrochemistry (IAU Symp. 120), ed. M.S. Vardya and S.P. Tarafdar (D. Reidel), in press (1986).
4. "Interstellar Molecules and Astrochemistry", Turner, B.E., and Ziurys, L.M., in Galactic and Extragalactic Radio Astronomy, ed. K. Kellerman and G. Verschurr (Springer-Verlag: Berlin, Heidelberg, and New York), submitted for publication.
5. "New Interstellar Detections: Implications for Shock Chemistry", Ziurys, L.M., and Turner, B.E., Astrochemistry (IAU Symp. 120), ed. S.P. Tarafdar and M.S. Vardya (Dordrecht: Reidel), in press.
6. "Observations of OCS and a Search for OC₃S in the Interstellar Medium, Matthews, H.E., MacLeod, J.M., Broten, N.W., Friberg, P. and Madden, S.C., Astrophys.J., in press (1986).
7. "Detections of ¹³C-Substituted C₃H₂ in Astronomical Sources",

- Madden, S.C., Irvine, W.M., and Matthews, H.E., Astrophys.J., submitted.
8. "Observational Astrochemistry", Irvine, W.M. and Hjalmarsen, A., Adv. Space Sci., submitted.
 9. "Chemical Abundances in Molecular Clouds", Irvine, W.M., Goldsmith, P.F., and Hjalmarsen, A. in Summer School on Interstellar Processes, ed. D. Hollenbach and H. Thronson (Dordrecht: Reidel), in press.
 10. "The C_3H_2 220-211 Transition: Absorption in Cold Dark Clouds", Matthews, H.E., Madden, S.C., Avery, L.W. and Irvine, W.M., Astrophys.J. (Letters), in press.
 11. "A Search for Interstellar H_3O^+ ", Wootten, A., Boulanger, F., Ziurys, L.M., Bogey, M., Combes, F., Encarnaz, P., and Gerin, M., Astron. Astrophys., in press.
 12. "Studies of Interstellar Vibrationally Excited Molecules", Ziurys, L.M., Snell, R.L., Erickson, N.R., and Turner, B.E., in Summer School on Interstellar Processes, ed. D. Hollenbach and H. Thronson (Dordrecht: Reidel), in press.
 13. "Exobiology in Earth Orbit; Tarter, J., DeFrees, D., Brownlee, D., Usher, D., Klein, H.P., and Irvine, W.M., Fifth ISSOL Meeting, Berkeley, CA., July, 1986.
 14. "Multitransition Studies of C_3H_2 ", Madden, S.C., Irvine, W.M., Matthews, H.E. and Avery, L.M., in Summer School on Interstellar Processes, ed. D. Hollenbach and H. Thronson (Dordrecht: Reidel), in press.

Future Plans

Active research will continue on the abundance and distribution of cyclopropenylidene in interstellar sources. Observing time has been granted on the 100 meter telescope operated by the Max-Planck-Institut für Radioastronomie in Germany. This will enable high spatial resolution observations of the strong 18 GHz transition to be made. In addition, the ratio of the 18 to the 21 GHz transition, which is predicted to be an indicator of density, will be studied in a variety of sources. Moreover, there has recently been a laboratory measurement of the rotational frequencies of deuterated C_3H_2 , and we will attempt to detect this important isotopic variant. Many other interstellar molecules show strong deuterium fraction-

ation, which can be used to investigate relevant reaction pathways. Further observations of ^{13}C -substituted C_3H_2 will also continue including a search for the less abundant (on-axis) variant.

Ziurys will continue to pursue radio astronomical studies of high temperature chemistry through the detection and study of new interstellar species, as well as observations of known molecules which are predicted to be indicators of processes at elevated temperatures. Specifically, studies will be carried out excited vibrational modes of HCO^+ , N_2H^+ , and CS ; of metal containing species such as MgH , CaH , CaOH , and MgOH ; and studies of additional new molecular neutrals and ions.

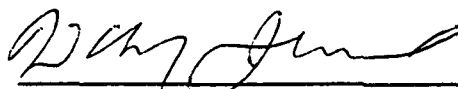
Madden is continuing her studies of highly excited masing transitions of ammonia in star forming regions. In an effort to determine the excitation process for the maser lines, additional transitions will be sought. A statistical equilibrium computer code is being developed to study the process of molecular excitation.

The assignment of presently unidentified interstellar lines will be continued through the search for related transitions and for satellite structure. In addition, a spectral line survey in the 20 GHz band has been allocated observing time at NRAO Green Bank and will be pursued by Irvine, Ziurys, Madden, and colleagues in Sweden and Canada.

Several observing projects described under Current Research will continue in order to better determine chemical abundances and relevant reaction processes. For example, studies of additional SO^+ transitions will be made, efforts to detect additional lines of PN to confirm the tentative identification will be pursued, and further observations in an attempt to confirm the identification of H_3O^+ will be undertaken. Likewise, Schloerb will continue study of the structure and kinematics of nearby molecular clouds in

order to study the process of star and solar nebula formation, and the resulting disruptive effects on the parental molecular clouds.

As a member of the Committee on Planetary Biology and Chemical Evolution (NAS-NRC) Irvine will be jointly responsible for the preparation of a strategy document for the study of Exobiology, which is being prepared for presentation to the Space Science Board. Irvine has also been invited by the Rector of Helsinki University to present an invited lecture on interstellar chemistry.



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